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A RATIONAL FUNCTION APPROXIMATION FOR THE INTEGRATION POINT IN EXPONENTIALLY WEIGHTED FINITE ELEMENT METHODS

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A rational function is presented for approximating the function f(z) = coth z - 1/z that appears in several exponentially fitted or weighted finite difference and finite element methods for convection-diffusion problems. The approximation is less expensive to evaluate than f(z) and provides greater accuracy than the doubly asymptotic approximation when z = 0(1).

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INTRODUCTION

Exponentially weighted Galerkin-finite element,[2,5,6] collocation,[4] and exponentially fitted finite difference[1,5,7] schemes have become popular and effective numerical methods for solving convection dominated convection-diffusion problems. They avoid the spurious mesh oscillations found in centered schemes at high values of the cell Reynolds or Peclet numbers and reduce the effects of numerical diffusion found in upwind finite difference schemes.

The exponential schemes all require evaluating the function

$$\xi = f(z) := \coth z - 1/z$$

in order to obtain their optimal accuracy. For example, the exponentially fitted Galerkin-finite element method for the two-point boundary value problem

$$\varepsilon \frac{d^2u}{dx^2} - c(x) \frac{du}{dx} = 0 \quad , \quad 0 < x < 1 \quad , \quad u(0) = A, \quad u(1) = B \tag{2}$$

on a uniform grid of spacing $h = 1/N$ is given by, (cf, e.g., Hughes[6])

$$(\varepsilon/h^2)(U_{i-1} - 2U_i + U_{i+1}) - (1/2h)[(1+\xi_i)c(\bar{x}_i)(U_i-U_{i-1}) + (1-\xi_i)c(\bar{x}_{i+1})(U_{i+1}-U_i)] = 0 \quad , \quad i = 1,2,\ldots,N-1 \tag{3a}$$

$$U_o = A \quad , \quad U_N = B \tag{3b,c}$$

Here U_i denotes the numerical approximation of $u(ih)$, $i = 0,1,\ldots,N$, $\bar{x}_i$ is some point on (x_{i-1}, x_i), e.g., the center of the subinterval, and ξ_i can be

*References are listed at the end of this report.

interpreted as a function evaluation point in a one-point quadrature rule (cf. Hughes[6]). The choice

$$\xi_i = f(\rho_i/2) \tag{4}$$

where ρ_i is the cell Reynolds or Peclet number

$$\rho_i = c(\bar{x}_i)h/\varepsilon \tag{5}$$

is known to give the exact solution of Eq. (2) for all ρ_i when c is a constant (cf. Christie et al.[2]).

The function f(z) is relatively expensive to evaluate because of the exponential functions and is usually replaced by the "doubly asymptotic" approximation

$$\xi = f_A(z) := \begin{cases} z/3 \;, & |z| < 3 \\ \mathrm{sgn}(z), & |z| > 3 \end{cases} \tag{6}$$

The function $f_A(z)$ provides an $O(z^3)$ approximation to f(z) when $|z| << 1$ and an $O(1/z)$ approximation when $|z| >> 1$. Furthermore, when Eq. (6) is used in Eq. (3) and c(x) is smooth, U_i provides an $O(\rho^4)$ approximation when

$$\rho := \max_{1<i<N} |\rho_i| \tag{7}$$

is small and an $O(1/\rho)$ approximation when ρ is large.

Thus, $f_A(z)$ provides a good approximation of f(z) when z is either small or large, but has large errors when z = O(1) (cf. Figure 1). The largest difference between f(z) and $f_A(z)$ is 0.328 and it occurs at z = 3. This corresponds to a value of $\rho = 6$ and since cell Reynolds numbers in this vicinity are reasonably common in computation it behooves us to find a better approximation for f(z) than $f_A(z)$ when z = O(1).

In this note, we consider rational function approximations having the form

$$\xi = f_R(z) := \frac{z(1 + \alpha|z|)}{3 + \beta|z| + \alpha z^2} \tag{8}$$

for appropriate choices of α and β. This approximation will be considered successful if it provides better accuracy than $f_A(z)$ and is still less expensive to evaluate than $f(z)$.

Like $f_A(z)$, we see that $f_R(z)$ correctly approximates $f(z)$ as $z \to 0$ and as $|z| \to \infty$ for all values of β and all $\alpha \neq 0$. The maximum difference between $f(z)$ and $f_R(z)$ is about 0.0115 for the nearly optimal values of $\alpha = 0.6$ and $\beta = 1.38$ (cf. Figure 1). Furthermore, when f, f_A, and f_R were evaluated for 1000 values of $z \in [0,100]$ we found that f_R took 35 percent less time to evaluate than f while f_A took 49 percent less time than f. The approximation f_R also provided greater accuracy than f_A for the computed solution U_i, $i = 0,1,\ldots,N$, of two model problems. The savings in time and improvement in accuracy are significant and may be especially important in multi-dimensional problems. As previously noted, the greatest gains occur when $\rho_i = O(1)$ and $c(x)$ is smooth.

RATIONAL FUNCTION APPROXIMATION

We will want to restrict α and β in Eq. (8) so that our approximation $f_R(z)$ satisfies the following three conditions:

i. $f_R(z)$ should be a good approximation of $f(z)$ when z is small and large, although not necessarily as good as $f_A(z)$.

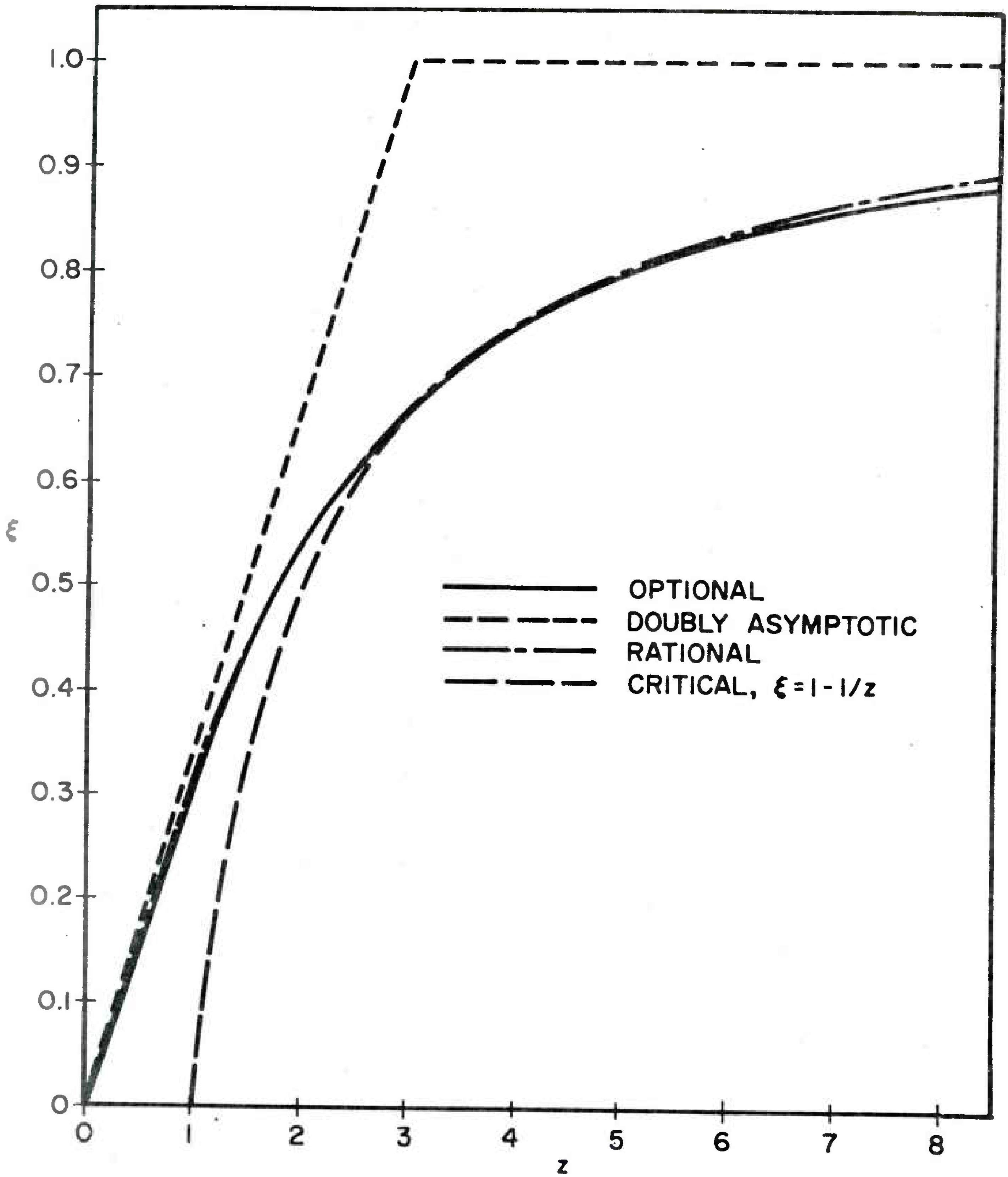

Figure 1. Optimal, doubly asymptotic, rational, and critical choices of $\xi = f(z)$ given by equations (1), (6), (8), and $\xi = 1 - 1/z$, respectively.

ii. The solution U_i of Eq. (3) should be oscillation free. Christie et al.[2] have shown that this will be the case when

$$\begin{aligned} z > 0 \quad &, \quad \xi \geq 1 - 1/z \\ z < 0 \quad &, \quad \xi \leq -(1 - 1/z) \\ z = 0 \quad &, \quad \text{all } \xi \end{aligned} \tag{9}$$

iii. Since $f(z)$ is a monotonically increasing function of z we ask that

$$\frac{df_R(z)}{dz} > 0 \quad , \text{all} \quad z \tag{10}$$

Since both $f(z)$ and $f_R(z)$ are odd functions of z it suffices to enforce these conditions for $z \geq 0$. We shall see that enough flexibility remains for us to select α and β to improve accuracy when $z = O(1)$.

The functions $f(z)$ and $f_R(z)$ have the following asymptotic behavior for small and large values of z:

$$f(z) = \begin{cases} \dfrac{z}{3} - \dfrac{z^3}{45} + \dfrac{2z^5}{945} + O(z^7) \quad , \quad z \ll 1 & \text{(11a)} \\[2ex] 1 - \dfrac{1}{z} + O(e^{-2z}) \quad , \quad z \gg 1 & \text{(11b)} \end{cases}$$

$$f_R(z) = \begin{cases} \dfrac{z}{3}\left[1 + (\alpha - \dfrac{1}{3}\beta)z + \dfrac{1}{3}(\dfrac{1}{3}\beta^2 - \alpha\beta - \alpha)z^2 + O(z^3)\right], \quad z \ll 1 & \text{(12a)} \\[2ex] 1 - \dfrac{\beta-1}{\alpha z} + \dfrac{\beta^2-\beta-3\alpha}{\alpha^2 z^2} + O(\dfrac{1}{z^3}) \quad , \quad z \gg 1 \quad , \quad \alpha \neq 0 & \text{(12b)} \\[2ex] \dfrac{1}{\beta}\left[1 - \dfrac{3}{\beta z} + \dfrac{9}{\beta^2 z^2} + O(\dfrac{1}{z^3})\right] \quad , \quad z \gg 1, \ \alpha = 0 \quad , \quad \beta \neq 0 & \text{(12c)} \end{cases}$$

Equation (12c) only gives the correct limiting value of $f(z)$ as $z \to \infty$ when $\beta = 1$ and this value of β does not satisfy Eq. (9); hence, we will no longer consider approximations with $\alpha = 0$.

Let

$$e(z) := f_R(z) - f(z) \tag{13}$$

denote the pointwise error and use Eqs. (11) and (12) to obtain

$$e(z) = \begin{cases} (\alpha - \frac{1}{3}\beta)\frac{z^2}{3} + (\frac{1}{3}\beta^2 - \alpha\beta - \alpha + \frac{1}{5})\frac{z^3}{9} + O(z^4) & , \quad z \ll 1 \\ (1 - \frac{\beta-1}{\alpha})\frac{1}{z} + \frac{\beta^2-\beta-3\alpha}{\alpha^2 z^2} + O(\frac{1}{z^3}) & , \quad z \gg 1 \end{cases} \tag{14}$$

We see that the rate of convergence as $z \to 0$ can be improved from $O(z^2)$ to $O(z^3)$ by selecting

$$\beta = 3\alpha \tag{15}$$

while the rate of convergence as $z \to \infty$ can be improved from $O(1/z)$ to $O(1/z^2)$ by selecting

$$\beta = 1 + \alpha \tag{16}$$

Both Eqs. (15) and (16) can be satisfied simultaneously by selecting $\alpha = 1/2$ and $\beta = 3/2$.

Before deciding on either or both of Eqs. (15) and (16) we still must find bounds on α and β so that Eqs. (9) and (10) are satisfied. It is slightly simpler to consider Eq. (10) first; thus, we differentiate Eq. (8) to obtain

$$\frac{df_R}{dz} = \frac{3 + 6\alpha z + \alpha z^2(\beta-1)}{(3+\beta z+\alpha z^2)^2} \quad , \quad z > 0 \tag{17}$$

For $df_R/dz > 0$, the polynomial

$$p(z) = 3 + 6\alpha z + \alpha z^2(\beta-1) \tag{18}$$

should not have any positive roots. It will have two negative roots if $\alpha > 0$ and $\beta > 1$ and two complex roots if $\alpha > 0$ and $\beta > 1+3\alpha$ or $\alpha < 0$ and $\beta < 1+3\alpha$. For the reasons of accuracy expressed by Eqs. (15) and (16) we would like to be as close to $\alpha = 1/2$ and $\beta = 3/2$ as possible. Hence, we will not consider the region where $\alpha < 0$ and confine our attention to choices satisfying $\alpha > 0$ and $\beta > 1$.

Finally using Eq. (8), condition (9) will be satisfied if

$$f_R(z) - (1 - \frac{1}{z}) = \frac{3 + (\beta-3)z + (1+\alpha-\beta)z^2}{z^2(3+\beta z+\alpha z^2)} \geq 0 \quad , \quad z \geq 0 \tag{19}$$

Since α and β are positive we want the polynomial

$$p(z) = 3 + (\beta-3)z + (1+\alpha-\beta)z^2 \tag{20}$$

to have no positive roots. $p(z)$ will have two negative roots if $3 \leq \beta \leq 1+\alpha$ and two complex roots if

$$\beta < -3 + 2\sqrt{3(1+\alpha)} \tag{21}$$

The values of α and β that satisfy both Eqs. (9) and (10) are

$$\frac{1}{3} < \alpha \leq 3 \quad , \quad 1 < \beta < -3 + 2\sqrt{3(1+\alpha)}$$
$$\alpha > 3 \quad , \quad 1 < \beta < 1+\alpha \tag{22}$$

This region is shown shaded in Figure 2. Note that the point $\alpha = 1/2$, $\beta = 3/2$, which improves accuracy for small and large values of z, fails to satisfy condition (10). However, Figure 2 suggests that an effective alternative might be to pick the point on the curve $\beta = -3 + 2\sqrt{3(1+\alpha)}$ that is closest to $\alpha = 1/2$, $\beta = 3/2$. This point is $\alpha = 0.5931$, $\beta = 1.3723$ and a search shows that it is near the point which minimizes the maximum value of $|e(z)|$, for all z.

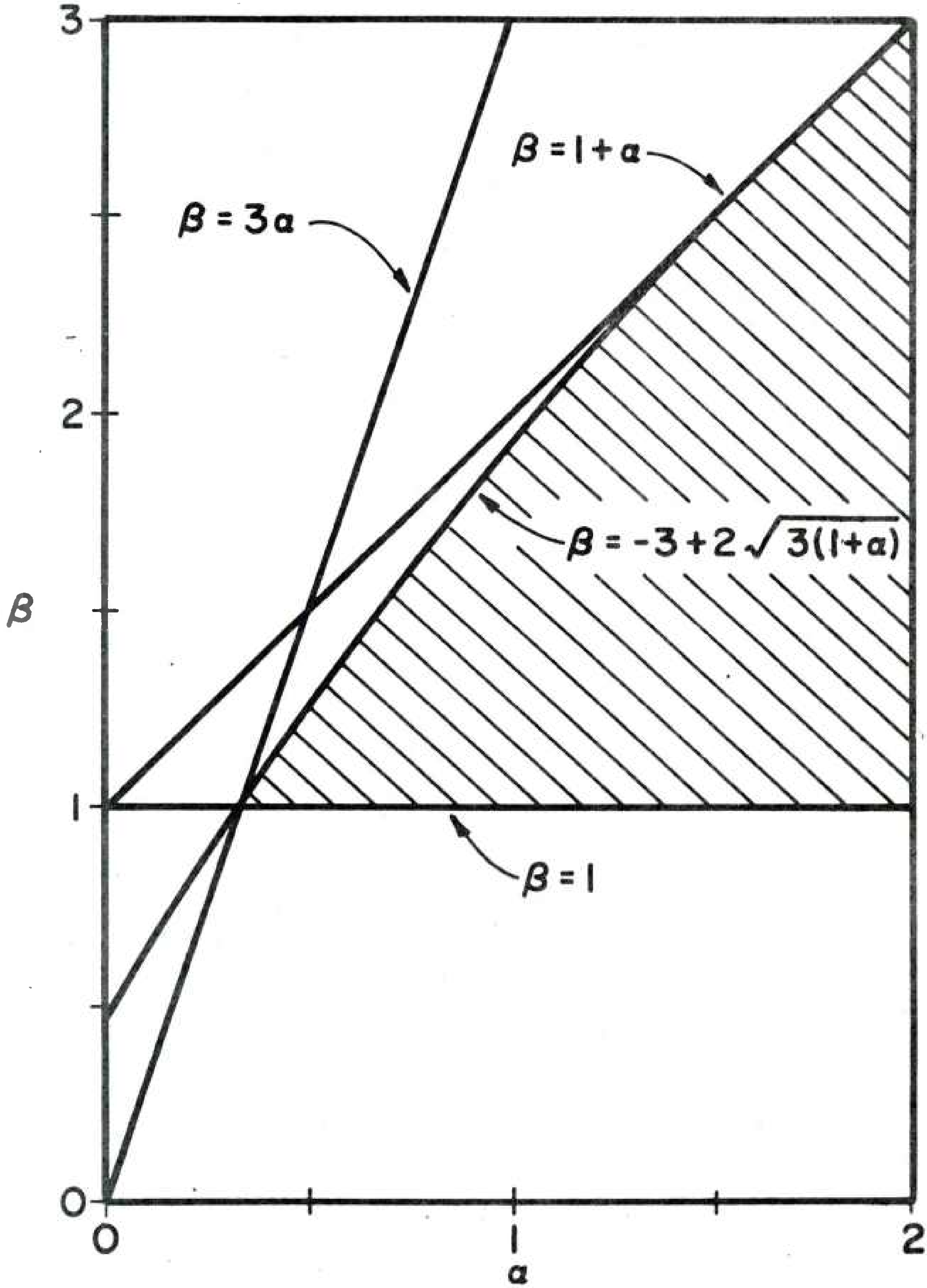

Figure 2. Region of acceptable values of α and β (shaded) that satisfies equations (9) and (10).

In the examples of the next section we used $\alpha = 0.6$ and $\beta = 1.38$ for which the maximum value of $|e(z)|$ is 0.0115.

NUMERICAL RESULTS

The approximations $f_A(z)$ and $f_R(z)$ and the exact function $f(z)$ given by Eqs. (6), (8), and (1), respectively, were coded in FORTRAN and used in the series of numerical experiments described below.

Equation (1) cannot be used for $f(z)$ when z is near zero and it was replaced by the expansion (11a) for $|z| \leqslant 0.01$. The FORTRAN Library function for tanh (z) was used in Eq. (1) when z was not small. All calculations were performed in double precision arithmetic on either an IBM 3033 at the Rensselaer Polytechnic Institute or an IBM 4341 at the Benet Weapons Laboratory.

In our first experiment, we evaluated $f(z)$, $f_A(z)$, and $f_R(z)$ for 1000 values of $z \in [0,100]$ and timed the results. The normalized times recorded in Table 1 were averaged over several runs and include only the times to evaluate the functions and neither input/output nor supervisor state times. Variations in times from run to run were less than two percent. The results indicate that f_R took 35 percent and f_A took 49 percent less time to evaluate than f. The relative timing figures can be expected to vary significantly from computer to computer and even from compiler to compiler; however, the differences between the times to evaluate f_R and f are large enough so that savings should be achieved in most environments.

TABLE 1. RELATIVE COMPUTER TIMES TO EVALUATE THE APPROXIMATIONS $f_A(z)$ AND $f_R(z)$ AND THE EXACT FUNCTION $f(z)$ FOR 1000 VALUES OF z ON $0 < z < 100$.

Method	Time
Doubly Asymptotic Approximation, Eq. (6)	0.508
Rational Approximation, Eq. (8)	0.654
Exact, Eqs. (1), (11a)	1.000

TABLE 2. MAXIMUM ERRORS AT STEADY STATE FOR EXAMPLE 1.

ρ	λ	Doubly Asymptotic	Lax Wendroff	Rational	Optimal
6	0.75	0.204×10^{-1}	0.159×10^{-2}	0.866×10^{-3}	0.250×10^{-13}
500	0.95	0.200×10^{-2}	0.235×10^{-1}	0.705×10^{-3}	0.208×10^{-11}

In order to study variations in the computed solutions when the different approximations of $f(z)$ are used we consider two boundary value problems having the form

$$\varepsilon \frac{d^2u}{dx^2} - \frac{dF(u)}{dx} = 0 \quad , \quad 0 < x < 1 \quad , \quad u(0) = A \quad , \quad u(1) = 0 \qquad (23)$$

Since our motivation for performing the work described in this note is to study exponentially weighted finite element schemes for transient problems[3] we do not use the numerical method (3) but rather, we follow Osher[8] and consider the solution of (23) as the steady state limit of the following initial-boundary value problem

$$\frac{\partial u}{\partial t} + \frac{\partial F(u)}{\partial x} = \varepsilon \frac{\partial^2 u}{\partial x^2} \quad , \quad 0 < x < 1 \quad , \quad t > 0 \qquad (24a)$$

$$u(0,t) = A \quad , \quad u(1,t) = 0 \quad , \quad u(x,0) = \begin{cases} A, & x = 0 \\ 0, & 0 < x \leq 1 \end{cases} \qquad (24b,c,d)$$

Equations (24) are approximated by the following explicit difference scheme

$$U_i^{n+1} = U_i^n - \lambda \, [(1+\xi_i)(F_i^n - F_{i-1}^n) + (1-\xi_i)(F_{i+1}^n - F_i^n)$$

$$+ (\varepsilon\lambda/h)(U_{i-1}^n - 2U_i^n + U_{i+1}^n) \quad , \quad i = 1,2,\ldots,N-1 \qquad (25a)$$

$$U_o^n = A \quad , \quad U_N^n = 0 \quad , \quad U_i^o = \begin{cases} 1, & i = 0 \\ 0, & i = 1,2,\ldots,N \end{cases} \qquad (25b,c,d)$$

where U_i^n denotes the numerical approximation of $u(ih,n\Delta t)$, Δt is the time step, and

$$\lambda = \Delta t/h \qquad (26)$$

The cell Reynolds number is still given by Eq. (5) with c defined as

$$c(x,t) = \frac{dF(u(x,t))}{du} \tag{27a}$$

and

$$\bar{x}_i = \begin{cases} x_i , & U_{i-1}^n + U_i^n < 0 \\ (x_{i-1}+x_i)/2 , & U_{i-1}^n + U_i^n = 0 \\ x_{i-1} , & (U_{i-1}^n+U_i^n) > 0 \end{cases} \tag{27b}$$

For reasons discussed in Flaherty and Mathon[4] these choices of $\bar{x}_i$ might be better than always using the center of the subinterval (x_{i-1},x_i).

The explicit difference scheme will be stable to linear perturbations provided that (cf. Osher[8] or Flaherty[3])

$$\lambda[c(\bar{x}_i,n\Delta t) + 2\varepsilon/h] < 1 \quad , \quad i = 1,2,\ldots,N, \; n \geq 0 \tag{28}$$

We use

$$E := \max_{1 \leq i \leq N} |u(ih,n\Delta t) - U_i^n| \tag{29}$$

with n chosen large enough so that steady state has been reached, to measure errors.

<u>Example 1</u>: Consider the constant coefficient problem for Eq. (23) with $F(u) = u$, $c = 1$, $A = 1$, which has the exact solution

$$u(x) = \frac{1 - e^{-(1-x)/\varepsilon}}{1 - e^{-1/\varepsilon}} \tag{30}$$

The results of calculations when ξ_i in Eq. (25) was evaluated by the doubly asymptotic approximation (6), the rational approximation (8), the Lax-Wendroff scheme ($\xi_i = \lambda$), and the optimal scheme (1) are presented in Table 2 for N = 20, $\rho = 6$, $\lambda = 0.75$, and N = 20, $\rho = 500$, $\lambda = 0.95$. The optimal scheme (1) is exact for this example. The samll errors reported in Table 2 are due to the combined effects of roundoff and our failure to reach the steady state limit. As expected the rational approximation improves upon the results of the doubly asymptotic approximation and the improvement is greatest for $\rho = 6$. The Lax-Wendroff solution oscillates when x is near unity.

Example 2. We consider the nonlinear Burgers' equation, $F(u) = u^2/2$ $c = u$, $A = \tanh 1/2\varepsilon$, for which the exact solution of Eq. (23) is

$$u(x) = \tanh(1-x)/2\varepsilon \tag{31}$$

Results comparing the doubly asymptotic, rational, and optimal choices of ξ_i are shown in Table 3 for N = 20, $\rho = h/\varepsilon = 6$, $\lambda = 0.75$, and N = 20, $\rho = 500$, $\lambda = 0.95$, and in Table 4 for $\varepsilon = 1/128$, $\rho = 1,2,4,8,16$. In Table 5 we show results for the error $|U_i^n - u(ih,n\Delta t)|$ at steady state and $x = ih = 0.875$, 0.9375 for $\varepsilon = 1/128$ and $\rho = 1,2,4,8,16$. The solution obtained using the doubly asymptotic approximation had mesh oscillations for $\rho = 8$ and $\lambda = 0.96$ so this calculation was rerun with $\lambda = 0.48$.

Although accuracy is not as good for this nonlinear example, the results generally parallel our findings for the linear problem. Table 5 shows that the rational and optimal choices of ξ_i are better than the doubly asymptotic choice at reducing the effects of numerical diffusion for cell Reynolds numbers in the range of 2 to 16.

TABLE 3. MAXIMUM ERRORS AT STEADY STATE FOR EXAMPLE 2.

ρ	λ	Doubly Asymptotic	Rational	Optimal
6	0.75	0.124	0.761×10^{-1}	0.766×10^{-1}
500	0.95	0.200×10^{-2}	0.135×10^{-2}	0.100×10^{-2}

TABLE 4. MAXIMUM ERRORS AT STEADY STATE FOR EXAMPLE 2 WITH $\varepsilon = 1/128$.

AN * DENOTES THAT $\lambda = 0.48$ FOR THIS CASE.

ρ	λ	Doubly Asymptotic	Rational	Optimal
16	0.96	0.605×10^{-1}	0.330×10^{-1}	0.308×10^{-1}
8	0.96	0.117*	0.599×10^{-1}	0.601×10^{-1}
4	0.96	0.110	0.940×10^{-1}	0.932×10^{-1}
2	0.6912	0.627×10^{-1}	0.627×10^{-1}	0.618×10^{-1}
1	0.4608	0.156×10^{-1}	0.157×10^{-1}	0.156×10^{-1}

TABLE 5. ERRORS AT $x = 0.875$ AND 0.9375 AT STEADY STATE FOR EXAMPLE 2 WITH $\varepsilon = 1/128$. AN * DENOTES THAT $\lambda = 0.48$ FOR THIS CASE.

		x = 0.875			x = 0.9375		
ρ	λ	Doubly Asymptotic	Rational	Optimal	Doubly Asymptotic	Rational	Optimal
16	0.96	0.605×10^{-1}	0.330×10^{-1}	0.308×10^{-1}			
8	0.96	0.131×10^{-1}*	0.244×10^{-3}	0.249×10^{-3}	0.117	0.599×10^{-1}	0.601×10^{-1}
4	0.96	0.741×10^{-4}	0.142×10^{-3}	0.122×10^{-5}	0.118×10^{-1}	0.366×10^{-2}	0.351×10^{-2}
2	0.6912	0.273×10^{-6}	0.182×10^{-6}	0.125×10^{-6}	0.523×10^{-3}	0.438×10^{-3}	0.372×10^{-3}
1	0.4608	0.288×10^{-7}	0.340×10^{-7}	0.238×10^{-7}	0.769×10^{-4}	0.835×10^{-4}	0.709×10^{-4}

CONCLUSION

We have shown that the rational function approximation (8) is an alternative to the doubly asymptotic approximation (6) of $f(z)$ that offers greater accuracy for about a 30 percent increase in cost. The approximation is most useful for cell Reynolds numbers in the range of one to ten.

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